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The lattice constant of quartz $11\bar{2}0$

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In an earlier report[1] one of us pointed out the possibility of using certain atomic planes in quartz as crystal lattices in X-ray spectroscopy. The lattice constants were calculated from earlier determinations of the lengths of the axes and the reflection power taken from crystallographic investigations of quartz. This determination is the first one in a series for the purpose of checking the calculations.

The work was carried out with a "tube spectrometer" in the usual manner. As a thorough description has been given previously[2], we will here only give data of interest with regard to this investigation. The crystal plate was 25 × 15 × 0.5 mm having the surface 25 × 15 parallel to the atomic plane $11\bar{2}0$. The length of the tube was 372.21 ± 0.05 mm, and the width of the slit 0.015 mm. The X-ray tube, which was provided with an oxidecoated platinum filament and a copper target, was driven with 10 to 15 mA at 20 kV. The time of exposure was in the first order 15 minutes, in the second 30. The intensity in the second order is about half of that of the first.

The temperature was controlled at even intervals during each recording. The variations during a double exposure did not surmount 0.3° C.

The position of the tube was controlled after each exposure. Errors in the angular scale were eliminated by the fact that three different zero positions of the crystal were used, located 120° from each other. The results obtained from the recordings with the three different zero positions were in good agreement, which shows that the angular scale is correct.

The results are given in Tables 1 and 2. The notations are the following:

t = temperature;
$2\varphi_0$ = the angle obtained from reading the angular scale;
a = the distance between the $K\alpha_1$-lines of the double exposure;
$2\Delta\varphi$ = the angle computed from a and the tube length;
$\varphi_t = \varphi_0 + \Delta\varphi$ = the glancing angle at t° C;
$\Delta\varphi_t$ = the temperature correction of the glancing angle;
φ_{18} = the glancing angle at 18° C.

The temperature correction is obtained from the relation

$$\Delta\varphi_{t''} = 2.76\ (t - 18)\ \mathrm{tg}\ \varphi.$$

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[1] Brogren, G., Nova Acta Reg. Soc. Sci. Ups. Ser. IV. Vol. 14. N:o 4. 1949.

[2] Larsson, A., Phil. Mag. (7), 3, 1136, 1927.

Table 1

Cu Kα_1 in the first order.

Plate No.	$2\varphi_0$	a mm	$2\Delta\varphi$	φ_t	t	$\Delta\varphi_t$	φ_{18}
1	36° 26′ 58.3″	+0.6583	6′ 4.8″	18° 16′ 31.6″	20.8°	2.5″	18° 16′ 34.1″
2	39′ 52.1″	−0.7379	6′ 48.7″	31.7″	21.0°	2.7″	.4″
3	40′ 5.4″	−0.7634	7′ 3.0″	31.2″	21.3°	3.0″	.2″
4	21′ 59.6″	+1.1928	11′ 1.0″	30.3″	21.4°	3.1″	33.4″
5	26′ 15.8″	+0.7330	6′ 46.2″	31.0″	21.3°	3.0″	34.0″
6	11′ 56.1″	+2.2836	21′ 5.5″	30.8″	21.5°	3.2″	.0″
7	36′ 10.7″	−0.3374	3′ 6.8″	31.7″	20.9°	2.6″	.3″
8	38′ 16.7″	−0.5691	5′ 14.4″	31.2″	21.0°	2.7″	33.9″
9	37′ 58.7″	−0.5330	4′ 55.4″	31.7″	21.1°	2.8″	34.5″
10	37′ 59.0″	−0.5342	4′ 56.0″	31.5″	21.4°	3.1″	.6″
11	39′ 2.4″	−0.6504	6′ 0.4″	31.0″	21.5°	3.2″	.2″
12	24′ 5.6″	+0.9672	8′ 56.0″	30.8″	21.4°	3.1″	33.9″
13	21′ 19.2″	+1.2670	11′ 42.1″	30.7″	21.4°	3.1″	.8″
14	26′ 2.6″	+0.7558	6′ 58.9″	30.8″	21.3°	3.0″	.8″
				Mean value			18° 16′ 34.1″

Table 2

Cu Kα_1 in the second order.

Plate No.	$2\varphi_0$	a mm	$2\Delta\varphi$	φ_t	t	$\Delta\varphi_t$	φ_{18}
21	77° 51′ 0.7″	−1.1266	10′ 24.4″	38° 50′ 18.2″	21.1°	6.9″	38° 50′ 25.1″
22	41′ 36.3″	−0.1091	1′ 0.5″	17.4″	21.2°	7.1″	25.0″
23	43′ 56.8″	−0.3585	3′ 18.8″	19.0″	21.3°	7.3″	26.3″
24	39′ 30.8″	+0.1220	1′ 7.6″	19.2″	21.2°	7.1″	26.3″
25	38′ 48.9″	+0.1898	1′ 45.2″	17.1″	21.4°	7.6″	24.7″
26	43′ 18.2″	−0.2948	2′ 48.7″	17.4″	21.6°	8.0″	25.4″
				Mean value			38° 50′ 25.5″

If BEARDEN's[1] value of the wavelength of the Kα_1 line of copper $\lambda = 1537.399$ X.U. is used, we obtain the following value of the lattice constant of the two first orders.

$$d_1 = 2451.233 \text{ X. U.}$$
$$d_2 = 2451.392 \text{ X. U.}$$

From the Bragg modified law,

$$n \cdot \lambda = 2d\left(1 - \frac{4d^2}{n^2} \cdot \frac{\delta}{\lambda^2}\right) \sin \varphi_n$$

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[1] BEARDEN, J. A. and SHAW, C. H., Phys. Rev. 48, 18, 1935.

where $d = \lim d_n =$ the real atomic distance and

$$\delta = 1 - \mu \qquad (\mu = \text{the index of refraction}),$$

we get

$$\delta = \frac{\dfrac{\sin \varphi_n}{n} - \dfrac{\sin \varphi_m}{m}}{\dfrac{1}{n \sin \varphi_n} - \dfrac{1}{m \sin \varphi_m}}.$$

Insert the values of φ_1, φ_2 and λ. Then

$$\delta = 0.859(4) \cdot 10^{-6}$$

$$\frac{\delta}{\lambda^2} = 3.63(6) \cdot 10^{-12}.$$

These results agree well with those obtained by LARSSON.[1]

Computing the real atomic distance d from the Bragg law by means of the value of $\frac{\delta}{\lambda^2}$, determined above, we get

$$d = 2451.445 \text{ X. U.}$$

Thus

$$\begin{array}{r} d_1 = 2451.233 \text{ X. U.} \\ d_2 = 2451.392 \text{ X. U.} \\ d_3 = 2461.421 \text{ X. U.} \\ \hline d_n = 2451.445 \text{ X. U.} \end{array}$$

The error of this determination is less than 0.025 X. U.

As a comparison it can be mentioned that, if the atomic distance is computed from the lattice constant of the atomic plane $10\bar{1}0$ ($d = 4246.02$ X. U.), we obtain for the atomic plane $11\bar{2}0$ $d = 2451.441$ X. U. The agreement between the two values is very good as the difference between them is much less than the limit of error.

We would like to express our sincere gratitude to Professor A. E. LINDH and to Professor P. OHLIN who have followed our investigations with the greatest interest and given us valuable help and advice.

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[1] LARSSON, A., l.c.

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